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Quantum corrections to the dynamics of the Bose-Einstein condensate in a double-well potential

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The dynamics of the Bose-Einstein condensate (BEC) in a double-well potential is often investigated under the mean-field theory (MFT). This works successfully for large particle numbers with dynamical stability. But for dynamical instabilities, quantum corrections to the MFT becomes important [Phys.Rev.A **64**, 013605(2001)]. Recently the adiabatic dynamics of the double-well BEC is investigated under the MFT in terms of a dark variable [Phys.Rev.A **81**, 043621(2010)], which generalizes the adiabatic passage techniques in quantum optics to the nonlinear matter-wave case. We give a fully quantized version of it using second-quantization and introduce new correction terms from higher order interactions beyond the on-site interaction, which are interactions between the tunneling particle and the particle in the well and interactions between the tunneling particles. If only the on-site interaction is considered, this reduces to the usual two-mode BEC.

Keywords: Bose-Einstein condensate; double-well potential

1. Introduction

The dynamics of the Bose-Einstein condensate (BEC) is often investigated under the mean-field theory (MFT), which provides a classical field equation for the nonlinear matter wave and is the classical limit of the quantum theory in large number limit. MFT works successfully in predicting experimental results as the particle numbers of BEC is very large, so the classical limit captures the essence. In the vicinity of a mean-field dynamical instability, however, the quantum correction to the MFT becomes important¹. They provide accurate predictions for the dynamics by combining the mean-field with the fluctuations. As most investigations are done under the MFT, it is interesting to look at their behavior under quantum corrections.

On the other hand, the analogy to quantum optics is noticed in investigating BEC, because of its macroscopic coherence that allows us to view it as a large atom. A recent example is the discovery of a dark variable for the double-well BEC by Ottaviani et al², which is a nonlinear matter-wave extension of Vitanov and

Shore's work³ of a two-state atom, where a dark variable is found by looking into the analogy between the optical two-state Bloch equation and the three-state stimulated Raman adiabatic passage (STRAP) equations⁴. They compose three variables analogous to the Bloch spin from the ground states of the two wells and the dark variable is found by comparing the equation of the three variables with the STRAP equation. The adiabatic splitting, transport and self-trapping of the double-well BEC are investigated using this dark variable² under the MFT. The STRAP can be utilized to transport BEC in multiple wells^{5–9}.

In the paper, we give a fully quantized version of the work of Ottaviani et al. We introduce further quantum corrections by including higher order interactions beyond the on-site interaction. If these quantum corrections are turned off, this model would reduce to the two-mode BEC widely used in quantum entanglement^{10–19}.

2. The on-site Interaction

In MFT, the two-mode approximation is applied to the GP equation and the dynamics of the double-well BEC² is

$$\mathcal{H} \begin{pmatrix} c_L \\ c_R \end{pmatrix} = i \frac{d}{dt} \begin{pmatrix} c_L \\ c_R \end{pmatrix}, \quad (1)$$

where the Hamiltonian is given by

$$\mathcal{H} = \begin{pmatrix} \epsilon_L + U_L |c_L|^2 & \Omega \\ \Omega & \epsilon_R + U_R |c_R|^2 \end{pmatrix}. \quad (2)$$

Introducing the field operator $\hat{\Psi}(\vec{r}, t)$, the Hamiltonian can be written as

$$\begin{aligned} \mathcal{H} &= \mathcal{H}_0 + \mathcal{H}_{int} \\ &= \int d^3r \hat{\Psi}^\dagger H_0 \hat{\Psi} \\ &\quad + \frac{g}{2} \int d^3r \hat{\Psi}^\dagger \hat{\Psi}^\dagger \hat{\Psi} \hat{\Psi}, \end{aligned} \quad (3)$$

where $H_0 = -\nabla^2/2m + V(\vec{r}, t)$ is the single particle Hamiltonian with $V(\vec{r}, t)$ the double-well potential and $g = 4\pi a_s/m$ is the nonlinear interaction parameter with a_s the s -wave scattering length. Only spatial degrees of freedom and two-body interactions are considered. Under the two mode approximation, where all modes are omitted except the condensate modes, the field operator can be expanded $\hat{\Psi}(\vec{r}, t) = \hat{a}_L(t) \phi_L(\vec{r}) + \hat{a}_R(t) \phi_R(\vec{r})$, where $\hat{a}_{L,R}$ and $\phi_{L,R}$ are the annihilation operator and the ground state of the left and the right well respectively. The overlap between the two ground states is neglected because it is small compared with the on-site part, $\phi_L^* \phi_R \ll |\phi_L|^2$. Now the second quantized Hamiltonian becomes

$$\begin{aligned} \mathcal{H} &= \epsilon_L \hat{a}_L^\dagger \hat{a}_L + \Omega \hat{a}_L^\dagger \hat{a}_R + \frac{U_0}{2} \hat{a}_L^\dagger \hat{a}_L^\dagger \hat{a}_L \hat{a}_L \\ &\quad + \epsilon_R \hat{a}_R^\dagger \hat{a}_R + \Omega \hat{a}_R^\dagger \hat{a}_L + \frac{U_0}{2} \hat{a}_R^\dagger \hat{a}_R^\dagger \hat{a}_R \hat{a}_R, \end{aligned} \quad (4)$$

with the parameters

$$\epsilon_{L,R} = \int d^3r \phi_{L,R}^* H_0 \phi_{L,R}, \quad (5)$$

$$\Omega = \int d^3r \phi_L^* H_0 \phi_R = \int d^3r \phi_R^* H_0 \phi_L, \quad (6)$$

$$U_0 = g \int d^3r |\phi_L|^4 = \int d^3r |\phi_R|^4. \quad (7)$$

with $\epsilon_{L,R}$ the chemical potential of the two wells respectively and U_0 the nonlinear on-site interaction between particles in the same well. The tunneling rate Ω between the two wells is negative, but it can also be defined to be positive by adding corresponding minus signs in the Hamiltonian.

It is convenient to rewrite the Hamiltonian by the Schwinger angular momentum operators $\hat{J}_x = (\hat{a}_R^\dagger \hat{a}_L + \hat{a}_L^\dagger \hat{a}_R)/2$, $\hat{J}_y = (\hat{a}_R^\dagger \hat{a}_L - \hat{a}_L^\dagger \hat{a}_R)/2i$, $\hat{J}_z = (\hat{a}_R^\dagger \hat{a}_R - \hat{a}_L^\dagger \hat{a}_L)/2$, where $\hat{J}_{x,y}$ corresponds to the correlation between the two wells and \hat{J}_z is the particle number difference between the two wells. The Hamiltonian under these angular momentum operators becomes

$$\begin{aligned} \mathcal{H} &= \frac{E}{2}N + \epsilon \hat{J}_z + 2\Omega \hat{J}_x + U_0 \left(\hat{J}_z^2 + \frac{N^2}{4} - \frac{N}{2} \right) \\ &= U_0 \hat{J}_z^2 + \epsilon \hat{J}_z + 2\Omega \hat{J}_x, \end{aligned} \quad (8)$$

with $N = N_L + N_R$ the total particle number, $E = \epsilon_L + \epsilon_R$ the sum of the two chemical potentials and $\epsilon = \epsilon_R - \epsilon_L$ the difference of the two chemical potential. Terms containing N and E are assumed to be conserved and are neglected from the Hamiltonian. This is the often used Hamiltonian in quantum entanglement, which only the on-site interaction is included. The dynamics of the system manifests in the evolution of these angular momentum operators

$$\frac{d}{dt} \begin{pmatrix} \hat{J}_x \\ \hat{J}_y \\ \hat{J}_z \end{pmatrix} = \begin{pmatrix} -iU_0 & -(\epsilon + 2U_0 \hat{J}_z) & 0 \\ \epsilon + 2U_0 \hat{J}_z & -iU_0 & -2\Omega \\ 0 & 2\Omega & 0 \end{pmatrix} \begin{pmatrix} \hat{J}_x \\ \hat{J}_y \\ \hat{J}_z \end{pmatrix}. \quad (9)$$

Equation “Eq. (9)” is the second quantized version of the dynamics given in Ref. 2, where it is described by the evolution equation of the Bloch spin vector²⁰,

$$\frac{d}{dt} \begin{pmatrix} \mu \\ \nu \\ \omega \end{pmatrix} = \begin{pmatrix} 0 & -(\epsilon + U\omega) & 0 \\ (\epsilon + U\omega) & 0 & -2\omega \\ 0 & 2\omega & 0 \end{pmatrix} \begin{pmatrix} \mu \\ \nu \\ \omega \end{pmatrix}, \quad (10)$$

The elements of the Bloch spin vector μ, ν and ω are composed from the two modal populations.

The two evolution equations would resemble each other with the angular momentum operator corresponding to the Bloch spin vector, if we normalize the angular momentum operator by $N/2$, $2\hat{J}_{x,y,z}/N \sim u, v, w$. The nonlinear interaction parameter becomes $g = 4\pi N a_s / 2m$ under this normalization, which becomes the same

g in “Eq. (10)”. Without the normalization, the adiabatic splitting, transport and self-trapping can be given by the motion of the angular momentum operator on the Bloch sphere with radius $j = N/2$, while in Ref. 2 it corresponds to the motion of the Bloch spine in the unit sphere. The adiabatic transport corresponds to the variance of J_z from $-N/2$ to 0 then to $N/2$ and the self-trapping corresponds to its variance from $-N/2$ to 0 then back to $N/2$.

Except the resemblance of their appearance, these two equations are quite different. The first one is the quantized version of the second one and it is the evolution equation for quantum operators rather than classical variables. We can approximate the operators with their expectation values, with the lowest-order approximation corresponding the MFT and the second-order approximation corresponding to the equation given by Ref. 1. Also two diagonal terms of $-iU_0$ emerge in the quantized version, which puts a phase factor to J_x and J_y . So the phases are also important in the dynamics. The phases and particle numbers can be investigated under the mean field approximation²¹, where they exhibit oscillations in the phase space. In the angular momentum space, we can choose the eigenstates of \hat{J}_z as the basis set $\{|jm\rangle\}$. The state of the system at time t is given by $|\Psi(t)\rangle = \exp\{-iHt\}|\Psi_0\rangle$, where $|\Psi_0\rangle = |\frac{N}{2}, \frac{N}{2}\rangle$ is the initial state with the left well population. The adiabatic transport of the system then means the evolution from $|\Psi_0\rangle$ to $|\Psi(t)\rangle = |\frac{N}{2}, \frac{N}{2}\rangle$.

3. Higher Order Interactions

The above quantized version of Ref. 2 only includes the nonlinear effects up to the on-site interaction. It would be interesting to investigate the effects of the neglected interactions, which becomes useful when its behavior is investigated under a wide parameter regime. To do this, we add to the Hamiltonian “Eq. (4)” the overlapping part $\phi_L^* \phi_R$ and introduce two new parameters U_t and U_{tt} to describe their effects, where U_t captures interactions between the tunneling particle and the on-site particle and U_{tt} captures interactions between the tunneling particles themselves. We term the tunneling particle as ‘tunnelier’ for simplicity. Now the full Hamiltonian is given by

$$\begin{aligned} \mathcal{H} = & \epsilon_L \hat{a}_L^\dagger \hat{a}_L + \Omega \hat{a}_L^\dagger \hat{a}_R + \frac{U_0}{2} \hat{a}_L^\dagger \hat{a}_L^\dagger \hat{a}_L \hat{a}_L \\ & + U_t \left(\hat{a}_L^\dagger \hat{a}_L^\dagger \hat{a}_L \hat{a}_R + \hat{a}_L^\dagger \hat{a}_R^\dagger \hat{a}_L \hat{a}_L \right) + \frac{U_{tt}}{2} \left(\hat{a}_L^\dagger \hat{a}_L^\dagger \hat{a}_R \hat{a}_R + 2 \hat{a}_L^\dagger \hat{a}_R^\dagger \hat{a}_R \hat{a}_L \right) \\ & + \epsilon_R \hat{a}_R^\dagger \hat{a}_R + \Omega \hat{a}_R^\dagger \hat{a}_L + \frac{U_0}{2} \hat{a}_R^\dagger \hat{a}_R^\dagger \hat{a}_R \hat{a}_R \\ & + U_t \left(\hat{a}_R^\dagger \hat{a}_R^\dagger \hat{a}_R \hat{a}_L + \hat{a}_R^\dagger \hat{a}_L^\dagger \hat{a}_R \hat{a}_R \right) + \frac{U_{tt}}{2} \left(\hat{a}_R^\dagger \hat{a}_R^\dagger \hat{a}_L \hat{a}_L + 2 \hat{a}_R^\dagger \hat{a}_L^\dagger \hat{a}_L \hat{a}_R \right), \quad (11) \end{aligned}$$

with the newly introduced parameters given by $U_t = g \int d^3r |\psi_L|^2 (\psi_L^* \psi_R) = g \int d^3r |\psi_R|^2 (\psi_R^* \psi_L)$ and $U_{tt} = g \int d^3r (\psi_L^* \psi_R)^2 = g \int d^3r (\psi_R^* \psi_L)^2 =$

$g \int d^3r \psi_L^* \psi_R \psi_R^* \psi_L$. For simplicity reasons, we have assumed $\psi_L^* \psi_R = \psi_R^* \psi_L$. In the Schwinger representation, this Hamiltonian becomes

$$\begin{aligned} \mathcal{H} &= \frac{E}{2}N + \epsilon \hat{J}_z + 2\Omega \hat{J}_x + U_0 \left(\hat{J}_z^2 + \frac{N^2}{4} - \frac{N}{2} \right) \\ &\quad + 2U_t(N-1) \hat{J}_x + \frac{U_{tt}}{2} \left(\hat{J}_- \hat{J}_- + \hat{J}_+ \hat{J}_+ + 2 \left(\hat{J}_+ \hat{J}_- + \hat{J}_- \hat{J}_+ \right) - 2N \right) \\ &= \frac{E}{2}N + \epsilon \hat{J}_z + 2\Omega \hat{J}_x + U_0 \left(\hat{J}_z^2 + \frac{N^2}{4} - \frac{N}{2} \right) \\ &\quad + 2U_t(N-1) \hat{J}_x + U_{tt} \left(\hat{J}_x^2 - \hat{J}_y^2 - 2\hat{J}_z^2 + \frac{N^2}{2} \right) \\ &= (U_0 - 2U_{tt}) \hat{J}_z^2 + \epsilon \hat{J}_z + 2(\Omega + U_t(N-1)) \hat{J}_x + U_{tt} (\hat{J}_x^2 - \hat{J}_y^2). \end{aligned} \quad (12)$$

This representation illustrates the interactions between the tunneliers, with $\hat{J}_- \hat{J}_-$ the interaction between left tunneliers (particles tunneling from the right well to the left well), $\hat{J}_+ \hat{J}_+$ the interaction between the right tunneliers (particles tunneling from the left well to the right well), and $\hat{J}_+ \hat{J}_- + \hat{J}_- \hat{J}_+$ the interaction between the left tunnelier and the right tunnelier. We can see the modifications introduced to the Hamiltonian by comparing it with “Eq. (8)”. The interaction between the tunnelier and the on-site particle adds a term $U_t(N-1)$ to the original tunneling parameter Ω , the interaction between the left and the right tunneliers adds a term $-2U_{tt}$ to the original nonlinear on-site interaction parameter U_0 and the interaction of the left tunneliers and that of the right tunneliers add another nonlinear terms $U_{tt}(\hat{J}_x^2 - \hat{J}_y^2)$ to the whole Hamiltonian. The equation of motion of these operators is

$$\frac{d}{dt} \begin{pmatrix} \hat{J}_x \\ \hat{J}_y \\ \hat{J}_z \end{pmatrix} = \begin{pmatrix} -i(U_0 - U_{tt}) & -(\epsilon + 2(U_0 - U_{tt}) \hat{J}_z) & 0 \\ \epsilon + 2(U_0 - 3U_{tt}) \hat{J}_z & -i(U_0 - 3U_{tt}) & -2(\Omega + U_t(N-1)) \\ 0 & 2(\Omega + U_t(N-1) + 2U_{tt}\hat{J}_x) & -i2U_{tt} \end{pmatrix} \begin{pmatrix} \hat{J}_x \\ \hat{J}_y \\ \hat{J}_z \end{pmatrix}. \quad (13)$$

Compared with “Eq. (9)”, this equation is non-symmetric and there is even a phase term of \hat{J}_z . By the definition of \hat{J}_z , there is no phase term as the phases carried by $\hat{a}_{L,R}$ is canceled out in $\hat{a}_L^\dagger \hat{a}_L$ and $\hat{a}_R^\dagger \hat{a}_R$. The origin of this phase term of \hat{J}_z manifests in the commutation relationship of \hat{J}_x and \hat{J}_y , which is introduced in deriving this equation of motion from the Hamiltonian “Eq. (12)”.

In Ref. 2, the nonlinear parameter U_0 generates a rich adiabatic dynamics of the double-well BEC. Here the quantum corrections introduced by U_{tt} and U_t makes the dynamics even more complex. When U_{tt} and U_t are small compared with U_0 , the influence may not be very explicit; but when they are large enough, the formulations above would lose sense as the two-mode assumption no longer holds true. Numerical simulations are needed to investigate their influence to the dynamics under various parameter regimes.

4. Conclusion

We have obtained quantum corrections of higher order interactions for the quantized dynamics of the double-well BEC and given a fully quantized expression of it under the two-mode approximation. Two new parameters are obtained to express the influence of the interactions between the tunneling particle and the on-site particle and between the tunneling particles. So the dynamics of the double-well BEC becomes more rich under this quantized version. This allows numerical simulation for a wide range of parameter regime and new phenomenon may be obtained.

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